Ab Initio Calculations of Transport and Optical Properties of Aluminum and Silver

Dmitry Knyazev and Pavel Levashov [C, S]
Joint Institute for High Temperatures RAS, Moscow, Russia
pasha@ihed.ras.ru

This work is devoted to the *ab initio* calculation of dynamical electrical conductivity and optical properties of aluminum and silver. The calculation is performed using quantum molecular dynamics (QMD) and density functional theory (DFT). QMD simulation is used to calculate ionic trajectories. Independent ionic configurations are selected from the equilibrium section of the molecular dynamics run for the calculation of conductivity. Detailed zone structure calculation is performed for each of these configurations. Electronic energy levels and wave functions are obtained and then used to calculate the real part of dynamical electrical conductivity using the Kubo-Greenwood formula. The values of conductivity for different ionic configurations are averaged. The imaginary part of electrical conductivity is obtained via the Kramers-Kronig transformation. Then optical properties are calculated: complex dielectric function, complex refractive index, reflectivity and opacity. QMD simulation and electronic structure calculation are performed using Vienna *Ab initio* Simulation Package (VASP). The calculation is performed for aluminum and silver at different temperatures and densities in solid and liquid phase. Particular attention is devoted to the normal isochor for temperatures from normal up to 20000 K. The convergence of the results with the parameters of the calculation is examined. The results are compared with data of other authors, reference and experimental data. The calculations of this work were used to calibrate the semiempirical model of dielectric function, necessary for the simulation of femtosecond laser interaction with matter.